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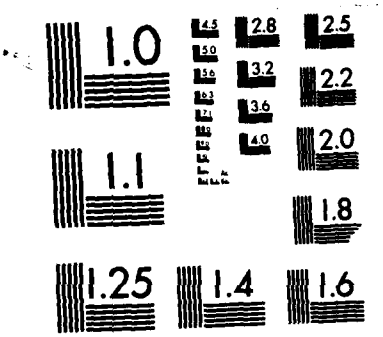

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Final Report for DAAG29-80-K-0044
GF 25517 - 6/15/80-5/15/84

CLUSTER VARIATION STUDY OF COHERENT ORDERING IN FCC AND BCC SOLID SOLUTIONS

Principal Investigator - Didier de Fontaine

PRIMARY OBJECTIVE

The primary objective of this investigaiton was the derivation of binary phase diagrams by means of a statistical mechanical model called the "Cluster Variation Method" (CVM). In particular, phase equilibrium as a function of the ratio $\alpha=V_2/V_1$ between the values of second and first neighbor effective pair interactions, α being the only physical input to the computer codes. The resulting phase diagrams are important for the purpose of analyzing experimentally determined alloy phase diagrams.

SUMMARY OF RESULTS

The calculated phase diagrams are called prototype ordering phase diagrams: "prototype" because no attempt was made initially to reproduce experimental diagrams of real alloy systems, "ordering" because only equilibrium between ordered superstructures and the parent lattice (in this case fcc) were investigated. The CVM was used in the so-called tetrahedron-octahedron approximation, which required considerable computer code development. It had been determined earlier that Bragg-Williams approximations were quite inadequate. The CVM, however, performed extremely well in those cases where a comparison could be made, for instance with Monte Carlo simulations.

The only input parameter was $\alpha=V_2/V_1$, the ratio of second to first-neighbor effective pair interactions in fcc cyrstals. These interactions suffice to stabilize certain ground states of order, many of which are experimentally found in real intermetallic compounds. Complete temperature - composition phase diagrams were obtained for seven values of α: 0.0, 0.25, 0.35, 0.45, 0.55, -0.2, -1.0. Hence, for the first time, an ordering prototype phase diagram with first and second neighbor interactions was derived for the fcc lattice with, as parameters, the temperature T, the average composition c, and the pair interaction ratio α. Along the way, the CVM technique was extended and computer codes developed, ground state analysis was generalized, and, importantly, CVM equations were developed to predict short-range order intensity in partially ordered systems.

The stated objectives of the original proposal were fully met, resulting in 16 publications (see attached list). In particular, Ref. 14, published as an "Overview" in Acta Metallurgica (1985), constitutes an extensive survey of work performed under the ARO(D) Contract. The text of this article is included in this final report.

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Phase Diagrams

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The primary objective of this investigation was the derivation of binary phase diagrams by means of a statistical mechanical model called the "Cluster Variation Method." In particular, phase equilibrium as a function of the ratio between the values of second and first neighbor effective pair interactions, the ratio being the only physical input to the computer codes. The resulting phase diagrams are important for the purpose of analyzing experimentally determined alloy phase diagrams.

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The work that has been accomplished can be regarded as an essential first step towards a general "Alloy Theory", i.e. one that would combine both electronic band structure and statistical thermodynamic calculations in one coherent whole, for the purpose of deriving phase diagrams from first principles. A new proposal was therefore submitted to ARO(D) with this objective in mind. As of this writing, the proposal is still in limbo, due, we are told, to lack of funds.

"Alloy theory" was the subject of the 1984 Physical Metallurgy Gordon Research Conference, under the Chairmanship of D. de Fontaine, and with ARO(D) financial backing. A report was sent to ARO(D) in late 1984 concerning this Conference.

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ORAL PRESENTATIONS

1. D. de Fontaine, "Coherent Phase Diagrams in the Cluster Variation Approximation," Alloy Theory and Development Workshop, Los Alamos, N. M., September 8-10, 1982.

2. D. de Fontaine, "First-Principles Phase Diagram Calculations, a Possibility?" Seminar at ALCOA, Pittsburgh, PA, Octobert 13, 1982.

3. D. de Fontaine, "First-Principles Phase Diagram Calculations, a Possibility?" Department Seminar at U. C. Berkeley, October 21, 1982.

4. J. M. Sanchez, B. Davies and D. de Fontaine, "Theoretical Study of Coherent Phase Equilibria in fcc Binary Systems," TMS-AIME 1983 Meeting, Atlanta, Georgia, March 6-10, 1983,

5. D. de Fontaine, "Ordering at Special and Not-So-Special Points," Seminar at Carnegie-Melon University, Pittsburgh, PA, March 11, 1983.

6. D. de Fontaine, "Composition Modulations in Solid Solutions," NATO Advanced Institute and the International Conference on Modulated Structure, Crete, Greece, June 27-30, 1983.

7. J. M. Sanchez, T. Mohri and D. de Fontaine, "Prototype Binary Phase Diagrams in the Cluster Variation Approximation," TMS-AIME 1984 Annual Meeting, Los Angeles, CA, February 26-March 1, 1984.

8. D. de Fontaine, "Prototype Ordering Phase Diagrams," High-Temperature Alloys: Theory and Design," Bethesda, Maryland, April 9-11, 1984.

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Dr. Winston Teitler	6/81 to 5/82	Programmer
Prof. D. de Fontaine	7/81, 7/82, 8/83	Prin. Investigator
Beverly Nagaue	11/81 to 2/82, 4/82, 7/82, 9/82	Clerical
Barrett Davis	3/82 to 6/82, 8/82, 11/82 to 3/83, 5/83 to 11/83	U. G. Coder
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Dr. Tetsuo Mohri	1/83 to 12/83	Post-Doc

BINARY ORDERING PROTOTYPE PHASE DIAGRAMS IN THE CLUSTER VARIATION APPROXIMATION

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ABSTRACT

The Tetrahedron Octahedron Cluster Variation Method (TO-CVM) has been employed to investigate fcc based order-disorder phase diagrams with first (positive) and second nearest neighbor pair interactions. The investigation covers the entire range of α values, the ratio of second to first nearest neighbor pair interactions. Ground state structures are discussed in detail and phase diagrams for seven different α values are presented. Good qualitative (topological features) and reasonable quantitative (transition temperatures) agreement is obtained with available Monte Carlo results, thereby confirm the reliability of the TO-CVM phase diagram calculations. The present study concludes the first global phase diagram investigation of fcc-based Ising model with first and second nearest neighbor pair interactions, and can be regarded as a precursor to more elaborate first principles phase diagram calculations.

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